

N -particle scattering matrix for electrons interacting on a quantum dot

A.V. Lebedev^{a,b}, G.B. Lesovik^b, and G. Blatter^a

^a*Theoretische Physik, Schafmattstrasse 32, ETH-Zürich, CH-8093 Zürich, Switzerland and*

^b*L.D. Landau Institute for Theoretical Physics, RAS, 119334 Moscow, Russia*

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We present a non-perturbative expression for the scattering matrix of N particles interacting inside a quantum dot. Characterizing the dot by its resonances, we find a compact form for the scattering matrix in a real-time representation. We study the transmission probabilities and interaction-induced orbital entanglement of two electrons incident on the dot in a spin-singlet state.

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The scattering matrix, taking asymptotically free incoming states through an interaction region and providing the free outgoing states, is of huge basic and practical interest. Originally introduced by Born [1] and by Wheeler and independently by Heisenberg [2] in atomic and particle physics, its application to electron transport [3] has made it into a central tool of mesoscopic physics [4]. Its formulation for non-interacting electrons provides the two-terminal conductance between reservoirs in terms of the transmission probability across the scatterer [3] and generalizations to complex setups [5] have been successful. Even more, the scattering matrix approach has been used to study noise [6] and a description of fluctuations in non-equilibrium situations is provided by the full counting statistics [7], with numerous applications known today [8]. These successes ask for a generalization to the interacting case [9], for which Goorden *et al.* [10] have recently derived the scattering matrix of two coupled conductors within a perturbative calculation.

Of generic interest in mesoscopic physics is the quantum dot, where the transport across is usually studied for a finite bias, and different approximate schemes have been used to include interactions in the transport analysis [11]. Recent interest concentrates on a new type of transport, where designed voltage pulses are generated to send a finite number of electrons towards the scattering region [12], see Ref. [13] for recent experiments in this direction. In this situation, novel effects, such as those due to particle exchange, show up quite prominently [14]. Moreover, this type of control on individual particles allows to study fundamental quantum properties such as the entanglement between electrons [15].

In this letter, we derive the N -particle scattering matrix for electrons that propagate freely in the leads but exhibit Coulomb repulsion when interacting on the dot. Within our formalism, the interaction is accounted for by the Hamiltonian $\hat{H}_{\text{int}} = e^2 \hat{N}^2 / 2C$, where \hat{N} is the dot's electron number operator and C denotes its capacitance. We use our results to study the wave function and degree of entanglement of two scattered electrons. Below, we construct the two-particle scattering matrix for the quantum dot including Coulomb interaction and generalize the result to the N -particle situation.

Usually, the scattering matrix connects states at given energies; here, we start with the propagator describing the scattering of wave packets in coordinate space. We start with a (properly symmetrized, spin indices are suppressed) incident two-electron wave function at time t_1 , $\Psi^{\text{in}}(\vec{y}, t_1)$, with $\vec{y} = \{y_1, y_2\}$. The scattered wave function at later times $t_2 > t_1$ can be obtained with the help of the two-particle propagator $K^{(2)}(\vec{x}, t_2; \vec{y}, t_1)$ describing the evolution of two particles from the initial positions \vec{y} at time t_1 to the final positions \vec{x} at t_2 ,

$$\Psi^{\text{out}}(\vec{x}, t_2) = \int d^2y K^{(2)}(\vec{x}, t_2; \vec{y}, t_1) \Psi^{\text{in}}(\vec{y}, t_1). \quad (1)$$

The two-particle propagator $K^{(2)}$ can be defined through a Feynman path integral over trajectories $\vec{x}(t)$,

$$K^{(2)}(\vec{x}, t_2; \vec{y}, t_1) = \int \mathcal{D}[\vec{x}] \exp\left(\frac{i}{\hbar} \int_{t_1}^{t_2} dt L^{(2)}(\vec{x}; \dot{\vec{x}})\right), \quad (2)$$

with the boundary conditions $\vec{x}(t_1) = \vec{y}$. Here, $L^{(2)}(\vec{x}, \dot{\vec{x}})$ is the system's Lagrangian including kinetic ($\propto m$), dot potential (U), and interaction ($\propto U_c = 2e^2/C$) energies,

$$L^{(2)} = \sum_{i=1}^2 \left[\frac{m\dot{x}_i^2}{2} - U(x_i) \right] - \frac{U_c}{4} [\chi_d(x_1) + \chi_d(x_2)]^2, \quad (3)$$

with the characteristic function $\chi_d(x)$ of the dot equal to unity within the dot and zero outside [16].

Without interaction, the two-particle propagator factorizes, $K^{(2)}(\vec{x}, t_2; \vec{y}, t_1) = \Pi_i K^{(1)}(x_i, t_2; y_i, t_1)$ with $K^{(1)}(x, t_2; y, t_1)$ the one-particle propagator, while the interaction mixes the particle trajectories. A Hubbard-Stratonovich transformation [17] with the real auxiliary field $z(t)$ allows us to decouple the quadratic interaction

$$K^{(2)}(\vec{x}, t_2; \vec{y}, t_1) = \int \mathcal{D}[z] \exp\left[i \frac{U_c}{\hbar} \int dt z^2(t)\right] \times K_{[z]}^{(1)}(x_1, t_2; y_1, t_1) K_{[z]}^{(1)}(x_2, t_2; y_2, t_1),$$

where $K_{[z]}^{(1)}(x, t_2; y, t_1)$ is the one-particle propagator in the presence of a fluctuating potential $U_c(t) = U_c z(t)$,

$$K_{[z]}^{(1)} = \int \mathcal{D}[x] \exp\left[\frac{i}{\hbar} \int_{t_1}^{t_2} dt \left(\frac{m\dot{x}^2}{2} - U(x) - U_c z(t) \chi_d(x) \right)\right].$$

Next, we introduce the scattering matrix $S_{\alpha\beta}^{(1)}(\varepsilon)$ of the dot in the absence of the fluctuating potential $U_c(t)$; the indices $\alpha, \beta \in \{\text{L,R}\}$ specify the lead indices for the outgoing (α) and incoming (β) scattering channels and ε denotes the energy variable. We describe the dot through the resonance positions (ϵ_j) and (identical) widths (Γ); the scattering matrix $S_{\alpha\beta}^{(1)}(\varepsilon)$ then takes the form

$$S_{\alpha\beta}^{(1)}(\varepsilon) = r_{\alpha\beta} + \sum_j \frac{i\Gamma/2}{\varepsilon - \epsilon_j + i\Gamma/2} s_{\alpha\beta}^{(j)}, \quad (5)$$

where the constant 2×2 matrices $r_{\alpha\beta}$ and $s_{\alpha\beta}^{(j)}$ can be found from the unitarity conditions. The Fourier transform provides the real time (τ) representation

$$S_{\alpha\beta}^{(1)}(\tau) = \delta(\tau)r_{\alpha\beta} + \theta(\tau) \sum_j \frac{\eta}{2} e^{-i\omega_j\tau} e^{-\eta\tau/2} s_{\alpha\beta}^{(j)}, \quad (6)$$

where $\eta = \Gamma/\hbar$ is the inverse dwell time, $\omega_j = \epsilon_j/\hbar$ is the resonance frequency, and $\delta(\tau)$, $\theta(\tau)$ are the usual δ - and Heaviside functions. The first term in Eq. (6) describes the reflection of a particle that has not penetrated into the dot, while the subsequent terms correspond to processes where the particle has spent a time τ inside the dot; the factor $e^{-i\omega_j\tau}$ describes the accumulated phase. The presence of the fluctuating potential $U_c(t)$ contributes an additional phase to the one-particle scattering matrix (6),

$$S_{\alpha\beta,[z]}^{(1)}(t_2, t_1) = S_{\alpha\beta}^{(1)}(t_2 - t_1) \exp\left(-\frac{i}{\hbar} \int_{t_1}^{t_2} U_c(t) dt\right), \quad (7)$$

where t_1 and t_2 denote the arrival and escape times of the particle (we assume escape amplitudes that

depend weakly on energy). The additional phase derives from the gauge transformation $\Psi_z(x, t) \rightarrow \Psi(x, t) \exp(-\frac{i}{\hbar} \int^t dt' U_c(t'))$; we neglect the scattering potential of size $\sqrt{U_c \hbar v / l_d} \sim U_c \sqrt{v\epsilon/\alpha c}$ arising at the dot's edge (see Ref. 18; here, l_d and ϵ denote the dot size and its dielectric constant, α is the fine structure constant). With a typical mesoscopic setup in mind, we assume velocities v of order of the Fermi velocity and energies larger than the Coulomb energy, $\varepsilon(k) \gg U_c$; with typical ratios $v/c \sim 10^{-2}$, we can safely ignore the fluctuation corrections in the dot potential $U(x)$.

Next, we express the propagator $K_{[z]}^{(1)}$ through the scattering matrix (7). To simplify matters, we linearize the spectrum, $\varepsilon(k) = \hbar vk$; a particle escaped out of the dot then never returns. In terms of trajectories, the scattering process involves three stages: *i*) the ballistic motion with velocity v towards the dot, *ii*) the dwell time in the dot, and, *iii*) the ballistic propagation away from the dot. We define the coordinates in the left ($x < 0$) and right ($x > 0$) leads with respect to the left ($x = 0^-$) and right ($x = 0^+$) dot boundaries and express the propagator $K_{[z]}^{(1)}$ through the scattering matrix (7), $K_{\alpha\beta,[z]}^{(1)}(x, t_2; y, t_1) = S_{\alpha\beta,[z]}^{(1)}(\tau, s)/v$, where $s = t_1 + |y|/v$ and $\tau = t_2 - |x|/v$ are the arrival and escape times of the particle to and from the dot; similar definitions ($s_i = t_1 + |y_i|/v$ and $\tau_i = t_2 - |x_i|/v$) apply to the two-particle scattering matrix, for which we write

$$S_{\alpha_1\alpha_2\beta_1\beta_2}^{(2)}(\tau_1, \tau_2; s_1, s_2) = S_{\alpha_1\beta_1}^{(1)}(\tau_1 - s_1) S_{\alpha_2\beta_2}^{(1)}(\tau_2 - s_2) \left\langle \exp\left\{-i\omega_c \left[\int_{s_1}^{\tau_1} dt z(t) + \int_{s_2}^{\tau_2} dt z(t)\right]\right\} \right\rangle, \quad (8)$$

and in terms of which the two-particle propagator (4) assumes the form $K^{(2)} = S^{(2)}/v^2$. Here, $\omega_c = U_c/\hbar$ and the average in Eq. (8) is taken with respect to the fluctuating Gaussian field $z(t)$. The latter is δ correlated in time, $\langle z(t_2)z(t_1) \rangle = (i/2\omega_c)\delta(t_2 - t_1)$ (the complex propagator in Eq. (4) generates an imaginary correlator for the real field $z(t)$) and thus the last factor in Eq. (8) can be explicitly averaged over with the result

$$S_{\alpha_1\alpha_2\beta_1\beta_2}^{(2)}(\tau_1, \tau_2; s_1, s_2) = \tilde{S}_{\alpha_1\beta_1}^{(1)}(\tau_1 - s_1) \tilde{S}_{\alpha_2\beta_2}^{(1)}(\tau_2 - s_2) \exp(-i\omega_c \tau_{12}/2), \quad (9)$$

where $\tilde{S}_{\alpha\beta}^{(1)}$ is the scattering matrix (6) with renormalized resonance frequencies $\tilde{\epsilon}_j = \epsilon_j + U_c/4$ and τ_{12} is the time the two particles spend together in the dot,

$$\tau_{12} = \frac{1}{2}(|\tau_1 - s_2| + |\tau_2 - s_1| - |\tau_1 - \tau_2| - |s_1 - s_2|).$$

This two-particle scattering matrix (9) is the key result of this Letter. All effects of Coulomb interaction are ac-

counted for by renormalized resonance energies due to self-interaction of individual electrons in the dot and an additional phase accumulated by the electrons during their simultaneous presence in the quantum dot.

An inverse Fourier transformation provides us with the energy representation

$$S_{\alpha_1\alpha_2\beta_1\beta_2}^{(2)}(\varepsilon'_1, \varepsilon'_2; \varepsilon_1, \varepsilon_2) = (2\pi)^2 \delta(\varepsilon_1 - \varepsilon'_1) \delta(\varepsilon_2 - \varepsilon'_2) S_{\alpha_1\beta_1}^{(1)}(\varepsilon_1) S_{\alpha_2\beta_2}^{(1)}(\varepsilon_2) + 2\pi \delta(\varepsilon_1 + \varepsilon_2 - \varepsilon'_1 - \varepsilon'_2) \times \sum_{jk} \frac{(iU_c/2) s_{\alpha_1\beta_1}^{(j)} s_{\alpha_2\beta_2}^{(k)}}{\varepsilon_1 + \varepsilon_2 - \tilde{\varepsilon}_j - \tilde{\varepsilon}_k - U_c/2 + i\Gamma} \frac{i\frac{\Gamma}{2}}{\varepsilon_1 - \tilde{\varepsilon}_j + i\frac{\Gamma}{2}} \frac{i\frac{\Gamma}{2}}{\varepsilon_2 - \tilde{\varepsilon}_k + i\frac{\Gamma}{2}} \left(\frac{1}{\varepsilon'_1 - \tilde{\varepsilon}_j + i\frac{\Gamma}{2}} + \frac{1}{\varepsilon'_2 - \tilde{\varepsilon}_k + i\frac{\Gamma}{2}} \right). \quad (10)$$

The first term describes the non-interacting process where particles scatter sequentially. The second term accounts for inelastic processes where only the total energy $E = \varepsilon_1 + \varepsilon_2$ is conserved. The Coulomb interaction generates additional poles at $E_{jk} = \tilde{\varepsilon}_j + \tilde{\varepsilon}_k + U_c/2 - i\Gamma$ involving the total energy E . These interaction-induced singularities cannot be obtained via a perturbative expansion for large $U_c \gg \Gamma$. For weak interaction $U_c \ll \Gamma$ or far away from the resonances $|E - \tilde{\varepsilon}_j - \tilde{\varepsilon}_k| \gg U_c$, the expansion of Eq. (10) to first order in U_c reproduces the perturbative result obtained in Ref. [10].

The above derivation for the two-particle scattering matrix can be generalized to N particles; the averaging over the field $z(t)$ generates an additional phase factor accounting for the pairwise interaction of particles residing simultaneously (for a time τ_{jk}) on the dot,

$$S_{\{\alpha_j\beta_j\}}^{(N)}(\{\tau_j; s_j\}) = \prod_{j>k}^N e^{-i\omega_c \tau_{jk}/2} \prod_{j=1}^N \tilde{S}_{\alpha_j\beta_j}^{(1)}(\tau_j - s_j).$$

The above result also holds true for a multichannel setup, with $\alpha_j, \beta_j, j = 1, \dots, N$ turning into multichannel indices. In particular, the results can be straightforwardly applied to the experimental setup [20] with two

parallel leads feeding/emptying two capacitively coupled dots that has been recently used to measure interaction-induced cross correlations, see also Ref. 10.

In applying our results to realistic mesoscopic problems, we have to avoid mixing between the scattered particles and the electrons in the Fermi sea. Hence, we do not consider situations with levels within the distance Γ around the Fermi energy ε_F and assume that U_c does not shift a level across ε_F ; the latter allows us to ignore complications due to the Kondo effect [19]. In the following, we study the scattering problem of two single-electron excitations created above the Fermi sea and a quantum dot with only one resonance at $\tilde{\varepsilon}_0$ above the Fermi energy ε_F , $\tilde{\varepsilon}_0 - \varepsilon_F \gg \Gamma$. The scattering matrix (10) then tells, that (the non-trivial component of) the scattered wave function involves energies near $\tilde{\varepsilon}_0$ and $\tilde{\varepsilon}_+ = \tilde{\varepsilon}_0 + U_c/2$.

We start from a two-electron state with wave function $\Psi^{\text{in}}(x_1, x_2)$ created at time $t = 0$ in the left lead and moving towards to the dot [21]. The scattered wave is given by Eq. (1) and can be expressed in terms of retarded variables $\xi_{1,2} = |x_{1,2}| - v_F t$, with v_F the Fermi velocity. The scattered wave to the right of the dot involving tunneling of both electrons assumes the form ($Y \equiv y_1 + y_2$)

$$\Psi_{\text{RR}}(\xi_1, \xi_2) = \frac{s_{\text{RL}}^2}{\ell^2} \left[e^{ik_+ \xi_>} e^{ik_0 \xi_<} \int_{\xi_>}^0 dy_1 dy_2 \Psi^{\text{in}}(y_1, y_2) e^{-ik_c(Y - |y_1 - y_2|)/2} e^{-ik_0 Y} e^{(\xi_1 + \xi_2 - Y)/\ell} \right. \\ \left. + e^{ik_0(\xi_1 + \xi_2)} \int_{\xi_<}^{\xi_>} dy_1 \int_{\xi_>}^0 dy_2 e^{-ik_0 Y} e^{(\xi_1 + \xi_2 - Y)/\ell} [\theta(\xi_2 - \xi_1) \Psi^{\text{in}}(y_1, y_2) + \theta(\xi_1 - \xi_2) \Psi^{\text{in}}(y_2, y_1)] \right], \quad (11)$$

where $\ell = 2\hbar/\Gamma v_F$ is the real-space width of the scattered wave, $\xi_> = \max\{\xi_1, \xi_2\}$, $\xi_< = \min\{\xi_1, \xi_2\}$, $k_0 = \tilde{\omega}_0/v_F$, $k_c = \omega_c/2v_F$, and $k_+ = k_0 + k_c$. The second term describes the process where the electrons do not overlap in the dot, while the term $\propto e^{ik_+ \xi_>} e^{ik_0 \xi_<}$ deals with the case where both electrons occupy the dot simultaneously during scattering. For electrons in a spin-triplet state with anti-symmetric orbital wave function $\Psi^{\text{in}}(y_1, y_2)$, this term vanishes and no interaction effects survive, a consequence of the Pauli principle.

Next, we choose a spin-singlet incoming state with one orbit ϕ , hence $\Psi^{\text{in}}(y_1, y_2) = \phi(y_1)\phi(y_2)$. To simplify mat-

ters, we choose an exponentially truncated plane wave function with a wave vector in resonance with the dot, $\phi(x) = \theta(a - x) e^{ik_0(x-a)} e^{(x-a)/2L} / \sqrt{L}$, where $a < 0$ is the initial position of the wave packet at $t = 0$ and L denotes its width; this choice allows to perform all integrals in Eq. (11) explicitly. We determine the probabilities P_1 and P_2 to transmit one and two electrons through the dot (at resonance, where $|s_{\text{RL}}| = 1$) and find them to depend only on the two dimensionless parameters $\alpha = k_c L$ and $\beta = \ell/2L$ quantifying the interaction and the resonance

width, respectively,

$$P_1 = \frac{2\beta}{1+3\beta} \left[\frac{2+3\beta}{(1+\beta)^2} - \frac{1}{(\alpha\beta)^2 + (1+\beta)^2} \right], \quad (12)$$

$$P_2 = \frac{1}{(1+3\beta)(1+\beta)^2} \left[1 + \beta(3+\beta) \times \frac{4(\alpha\beta)^2 + 3(\beta+3)(\beta+1)^2}{((\alpha\beta)^2 + (1+\beta)^2)(4(\alpha\beta)^2 + (3+\beta)^2)} \right]. \quad (13)$$

Without Coulomb interaction ($\alpha = 0$) or for vanishing dwell time ($\beta = 0$), we recover the results $P_1 = 2p(1-p)$ and $P_2 = p^2$, with $p = 1/(1+\beta)$ the single-particle tunnelling probability. Both, Coulomb interaction ($\alpha > 0$) and finite dwell time ($\beta > 0$) suppress the probability P_2 as compared with the non-interacting value p^2 . Even infinite Coulomb energy ($\alpha \rightarrow \infty$) still permits tunnelling of two electrons through the dot via sequential tunneling.

Finally, we show that the Coulomb interaction in the dot leads to an orbital entanglement of the two particles (for interaction-induced spin entanglement in a quantum dot, see Ref. 22). Here, we concentrate on the component of the wave function where two electrons are transmitted to the right and estimate its degree of entanglement, which is entirely due to the interaction in the dot. We analyze the situation where the length L of the incoming wave packet tends to zero, hence $\beta \rightarrow \infty$. In this case the normalized wave function on the right has the universal form (independent of Ψ^{in})

$$\Psi_{\text{RR}}(\xi_1, \xi_2) = (2/\ell) e^{ik_+\xi_1} e^{ik_0\xi_2} e^{(\xi_1+\xi_2)/\ell}, \quad (14)$$

where $\xi_{1,2} = x_{1,2} - a - v_F t < 0$. Eq. (14) describes a two-electron state with different momenta k_+ and $k_0 < k_+$, as has to be expected since the first electron escaping carries an energy shifted up by the Coulomb interaction. The state (14) can be rewritten in a form

$$\Psi_{\text{RR}} = (2/\ell) e^{i(k_0 + \frac{k_c}{2})(\xi_1+\xi_2)} e^{i\frac{k_c}{2}|\xi_1-\xi_2|} e^{(\xi_1+\xi_2)/\ell}, \quad (15)$$

reminding about the original Einstein-Podolsky-Rosen state with orbital entanglement [23]. To quantify its entanglement, one may calculate the von Neumann entropy E of the reduced density matrix $\rho(x, x') = \int dx_2 \Psi_{\text{RR}}(x, x_2) \Psi_{\text{RR}}^*(x', x_2)$. Instead, we determine the purity $\Pi(\rho) = \text{tr} \rho^2$, which is unity for separable states and provides the lower limit $E > 1 - \Pi$. With $A \equiv ik_c\ell/(2 - ik_c\ell)$, we find the density matrix

$$\begin{aligned} \rho(\xi, \xi') &= (2/\ell) \theta(-\xi) \theta(-\xi') e^{(\xi+\xi')/\ell} e^{ik_0(\xi-\xi')} \\ &\times [1 + A \theta(\xi-\xi') (e^{2\xi/\ell} - e^{ik_c(\xi-\xi')}) e^{2\xi'/\ell} \\ &+ A^* \theta(\xi'-\xi) (e^{2\xi'/\ell} - e^{ik_c(\xi-\xi')}) e^{2\xi/\ell}], \end{aligned} \quad (16)$$

that results into a purity $\Pi = [1 + 2/(1 + (k_c\ell/4)^2)]/3$. We conclude that at finite U_c the state (15) is entangled and the degree of entanglement saturates as the Coulomb interaction becomes larger than the resonance

width, $k_c\ell = U_c/\Gamma \gg 1$, i.e., when the energies of the escaped particles become distinguishable.

In conclusion, our expression for the multi-particle scattering matrix accounts for the redistribution of particle energies during inelastic scattering with the appearance of new resonance poles that cannot be obtained perturbatively for large $U_c \gg \Gamma$. As an application, we have studied the case where two electrons are transmitted across a dot with a single resonance and have investigated the ensuing orbital entanglement and the reduction in the two-particle transmission due to the interaction.

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